MATERIAL SAFETY DATA SHEET

1. SUBSTANCE AND SOURCE IDENTIFICATION

National Institute of Standards and Technology
Standard Reference Materials Program
100 Bureau Drive, Stop 2320
Gaithersburg, Maryland 20899-2320

SRM Number: 1494
MSDS Number: 1494
SRM Name: Aliphatic Hydrocarbons in 2,2,4-Trimethylpentane
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Description: Standard Reference Material (SRM) 1494 is a solution of 20 compounds, including even and odd carbon number aliphatic hydrocarbons from *n*-decane to *n*-eicosane, even carbon number aliphatic hydrocarbons from *n*-eicosane to *n*-tetratriacontane, and pristine and phytane in 2,2,4-trimethylpentane (*iso*-octane). This SRM is intended primarily for use in the calibration of chromatographic instrumentation used for the determination of aliphatic hydrocarbons. A unit of SRM 1494 consists of five 2-milliliter ampoules, each containing approximately 1.2 mL of solution.

Substance: 2,2,-4 Trimethylpentane
Other Designations: **2,2,-4 Trimethylpentane** (iso-octane; isobutyltrimethylmethane; 2,4,4-trimethylpentane; trimethylpentane)

2. COMPOSITION AND INFORMATION ON HAZARDOUS INGREDIENTS

Component	CAS Number	EINECS	Concentration (%)
2,4,4-trimethylpentane	540-84-1	208-759-1	100

Index, R/S Phrases (EC): F, Xn, Xi, N; R11, R38, R50/53, R65, R67; S2, S9, S16, S29, S33, S60, S61, S62
See "Section 15".

3. HAZARD IDENTIFICATION

Major Health Hazards: Respiratory tract irritation, aspiration hazard, central nervous system depression.
Physical Hazards: Extremely flammable liquid and vapor. Vapor may cause flash fire.
Potential Health Effects:

Inhalation: Respiratory irritation, nausea, difficulty breathing, headache, drowsiness, dizziness, loss of coordination.

Skin absorption: Headache, drowsiness, dizziness, loss of coordination.

Eye contact: Irritation.

Ingestion: Diarrhea, difficulty breathing, headache, drowsiness, dizziness, loss of coordination, lung congestion, aspiration.

Carcinogen Status:	Yes	No
National Toxicology Program (NTP) Report on Carcinogens		X
International Agency for Research on Cancer (IARC) Monographs		X
Occupational Safety and Health Administration (OSHA)		X

4. First Aid Measures

Skin Contact: Rinse affected area with soap and water for at least 15 minutes while removing contaminated clothing. Obtain medical assistance if necessary.
Eye Contact: Immediately flush eyes, including under the eyelids, with copious amounts of water for at least 15 minutes. Obtain medical assistance immediately.
Inhalation: If adverse effects occur, remove to uncontaminated area. If not breathing, give artificial respiration by qualified personnel. Get immediate medical attention.
Ingestion: Aspiration hazard. **DO NOT** induce vomiting. If vomiting occurs, keep head lower than hips to help prevent aspiration. Get immediate medical attention. If not breathing, give artificial respiration by qualified personnel.

5. Fire Fighting Measures

Fire and Explosion Hazards: Severe fire hazard. The vapor is heavier than air. Vapors or gases may ignite at distant ignition sources and flash back. Vapor/air mixtures are explosive above flash point.
Extinguishing Media: Regular dry chemical, carbon dioxide, water, regular foam.
Fire Procedures: Do not touch spilled material. Move container from fire area if it can be done without risk. Cool containers with water spray until well after the fire is out. Use extinguishing agents appropriate for surrounding fire. Keep unnecessary people away, isolate hazard area and deny entry.

Flash Point (°C): –12 **Autoignition (°C):** 415

Flammability Limits in Air (Volume %): **UPPER:** 6.0
LOWER: 1.1

Flammability Class (OSHA): IB

6. Accidental Release Measures

Occupational Release: Avoid heat, flames, sparks, and other sources of ignition. Absorb with sand or other non-combustible material.
Environmental Precautions: See "Section 13".
Clean-up Methods: Collect spilled material in appropriate container for proper disposal.

7. Handling and Storage

Storage: Store and handle in accordance with all current regulations and standards. Keep separated from incompatible substances. Store in a cool, dry place. Store in a well-ventilated area.
Precautions for Safe Handling: See "Section 8".

8. Exposure Controls and Personal Protection

Hazardous Component	Nominal Concentration (%)	Exposure Limits and Toxicity Data
2,2,4-Trymethylpentane	100	LD_{50} (Oral-Rat): > 5 g/kg

Engineering: An eye wash station and drench shower should be readily available near the handling and use areas.
Ventilation: Local exhaust ventilation system.
Respirator: Under conditions of frequent use or heavy exposure, if engineering controls are not feasible, respirator protection is required, see 42CFR84 for selection and use.
Eye Protection: Wear safety goggles. **DO NOT** wear contact lenses in the laboratory.
Personal Protection: Wear safety goggles and chemically resistant gloves and clothing.

9. PHYSICAL AND CHEMICAL PROPERTIES

2,2,4-Trimethylpentane	
Appearance and Odor: clear liquid, gasoline odor	**Specific Gravity (water = 1):** 0.692
Molecular Formula: $(C\text{-}H_3)_2\text{-}C\text{-}H\text{-}C\text{-}H_2\text{-}C\text{-}(C\text{-}H_3)_3$	**Volatility(%):** 100
Relative Molecular Mass: 114.23	**Water Solubility:** immiscible
Boiling Point (°C): 99	**Solvent Solubility:** ether, alcohol, acetone, benzene, toluene, chloroform, xylene, carbon disulfide, carbon tetrachloride, dimethylformamide, oils
Freezing Point (°C): –107	
Vapor Density (air = 1): 3.9	

10. STABILITY AND REACTIVITY

Stability: **X** **Stable** ____ **Unstable**

Stable at normal temperature and pressure.

Conditions to Avoid: Avoid heat, flames, sparks and other sources of ignition. Containers may rupture or explode if exposed to heat. Keep out of water supplies and sewers.

Incompatibility (Materials to Avoid): Oxidizing materials and reducing agents.

Hazardous Decomposition or Byproducts: Thermal decomposition produces oxides of carbon.

Hazardous Polymerization: ____ **Will Occur** **X** **Will Not Occur**

11. TOXICOLOGICAL INFORMATION

Route of Entry: **X** **Inhalation:** **X** **Skin** **X** **Ingestion**

Health Hazards (Acute): Inhalation exposure may cause irritation of the mucous membranes, rapid breathing, dizziness, fatigue, headache, light-headedness, lack of coordination, nausea, narcosis, and other central nervous system effects. Pulmonary damage may occur if aspirated into the lungs and may be fatal. Ingestion symptoms may include coughing, difficulty breathing, cyanosis, and pulmonary edema. May cause diarrhea, difficulty breathing, fatigue and slight central nervous system depression.

Medical Conditions Generally Aggravated by Exposure: Not applicable.

12. ECOLOGICAL INFORMATION

Adverse Effects: Not applicable.

13. DISPOSAL CONSIDERATIONS

Waste Disposal: Dispose in accordance with federal, state and local regulations. Keep out of water supplies and sewers.

14. TRANSPORTATION INFORMATION

DOT Registry: Octanes; Class Hazard 3; ID No. UN1262

15. REGULATORY INFORMATION

U.S. REGULATIONS

SARA TITLE III SARA SECTIONS 311/312 HAZARDOUS CATEGORIES (40 CFR 370.21):

ACUTE: Yes
CHRONIC: No
FIRE: Yes
REACTIVE: No
SUDDEN RELEASE: No

EC CLASSIFICATION

F	Highly Flammable
Xn	Harmful
Xi	Irritant
N	Dangerous for the Environment

EC RISK AND SAFETY PHRASES

R11	Highly flammable.
R38	Irritating to skin.
R50/53	Very toxic to aquatic organisms; may cause long-term. adverse effects in the aquatic environment.
R65	Harmful: may cause lung damage if swallowed.
R67	Vapors may cause drowsiness and dizziness.
S2	Keep out of reach of children.
S9	Keep container in a well-ventilated place.
S16	Keep away from sources of ignition - No smoking.
S29	Do not empty into drains.
S33	Take precautionary measures against static discharges.
S60	This material and/or its container must be disposed of as hazardous waste.
S61	Avoid release to the environment. Refer to special instructions/Safety data sheets.
S62	If swallowed, do not induce vomiting; seek medical advice immediately and show the container or label.

16. OTHER INFORMATION

Sources: MDL Information Systems, Inc., MSDS *2,2,4-Trimethylpentane,* 19 March 2003.

Disclaimer: Physical and chemical data contained in this MSDS are provided only for use as a guide in assessing the hazardous nature of the material. The MSDS was prepared carefully, using current references; however, NIST does not certify the data in the MSDS. The certified values for this material are given in the NIST Certificate of Analysis.